https://journals.aps.org/pre/abstract/10.1103/PhysRevE.103.033305

Tapia-Ruiz, Cernak & Elbert, **Phys. Rev. E 103**, 033305 (2021) – “Predicting nucleation using machine learning in the Ising model” link.aps.org

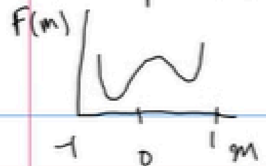
CNN and logistic-regression models trained on raw spin snapshots to approximate **p *B* (x)**; showed CNN remains accurate even near the spinodal.

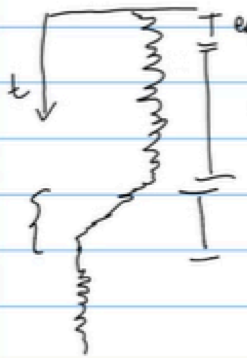
https://doi.org/10.1103/PhysRevE.103.033305
https://warwick.ac.uk/fac/sci/mathsys/courses/msc/mscprojects/projects_2019/david_quigley-px-nucleation_metrics.pdf
https://arxiv.org/abs/2310.08480
https://doi.org/10.1021/acs.jctc.3c00722

Rates of nucleation calculation

Time vs magnetization
Equilibriation time
Waiting time

Temp $T < T_c$; $h < 0$ small

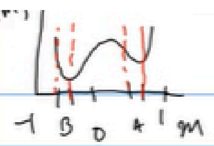




equilibration time

waiting time $\underbrace{t_w^{(1)}, t_w^{(2)}, \dots, t_w^{(m)}}$ - Transition Rate from

transition.



$t_w \gg t_{\text{transition}}$

equilibration time

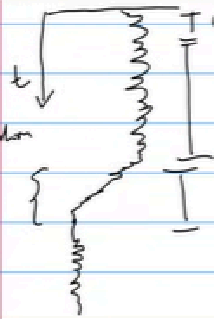
waiting time 1 $\underbrace{t_w^{(1)}, t_w^{(2)}, \dots, t_w^{(m)}}$ - Transition Rate from statistics

transition 2 Transition Paths Sampling

ML to get the transition Path Ensemble $\{ X_i^{[0,T]} \}_{i=1}^{P}$

Indicator fn. $h_A(X_i(t=0)) = 1 \longrightarrow \begin{cases} h_A(X) = 1 & \text{if } X \in A \\ \quad = 0 & \text{otherwise} \end{cases}$

$\begin{cases} h_B(X) = 1 & \text{if } X \in B \end{cases}$



T equilibration time

$t_w \gg t_{\text{transition}}$

waiting time (1) $\underbrace{t_w^{(1)}, t_w^{(2)} \ldots, t_w^{(M)}}$ – Transition Rate from statistics

transition (2) Transition Paths Sampling

ML to get the Transition Path Ensemble $\{ x_i^{[0,T]} \}_{i=1}^{P}$

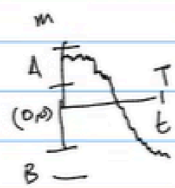
$A : m = [0.5, 0.6)$

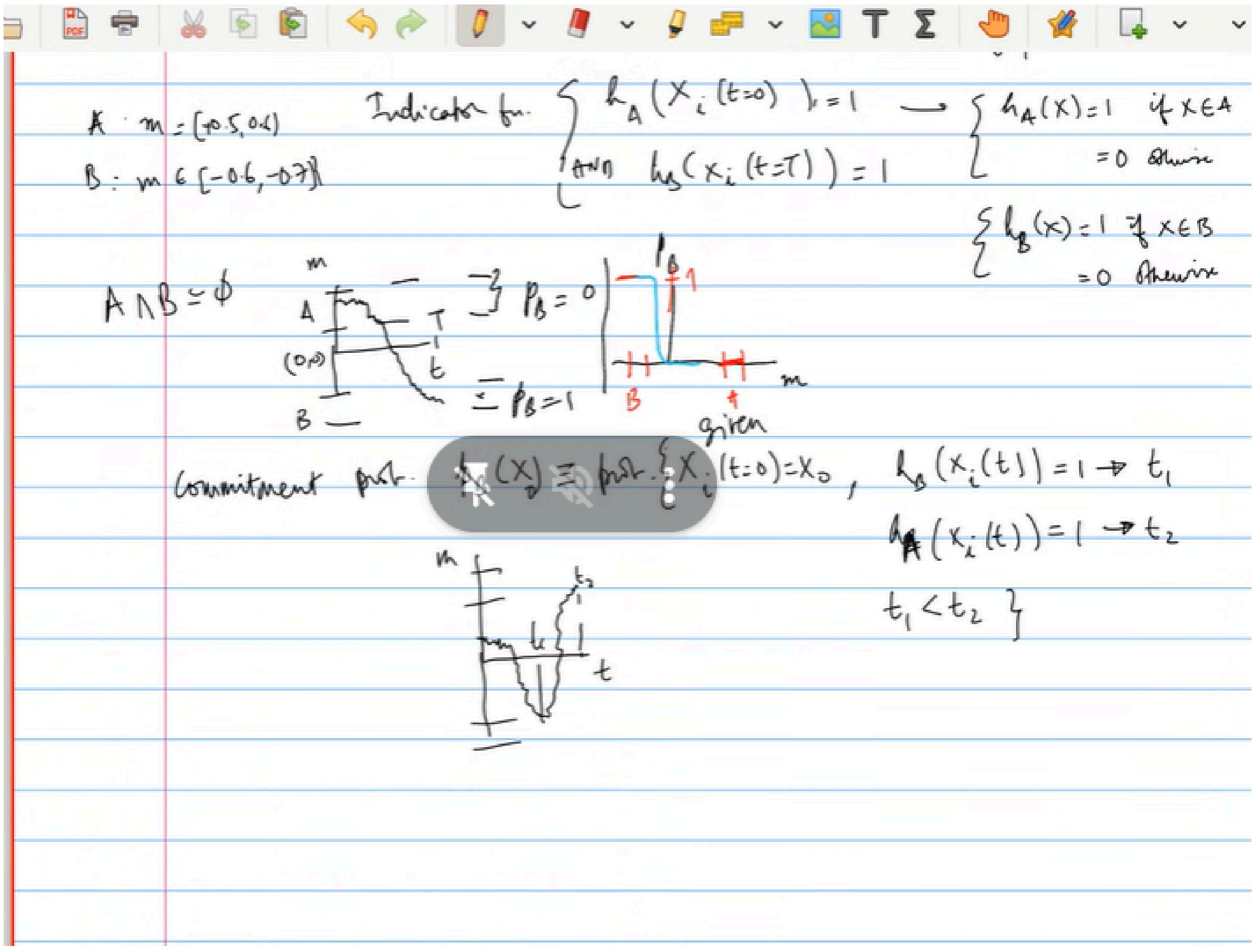
$B : m \in [-0.6, -0.7]$

Indicator fn. $\begin{cases} h_A(x_i(t=0)) = 1 \\ \text{AND } h_B(x_i(t=T)) = 1 \end{cases}$ $\longrightarrow$ $\begin{cases} h_A(x) = 1 & \text{if } x \in A \\ \quad = 0 & \text{otherwise} \end{cases}$

$\begin{cases} h_B(x) = 1 & \text{if } x \in B \\ \quad = 0 & \text{otherwise} \end{cases}$

$A \cap B = \phi$





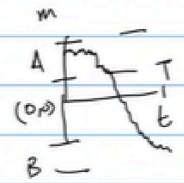
In the free energy minima all the config to the right will be 1 and all left will be 0, the problem is to catch the configurations in the abrupt switch,

https://www.nature.com/articles/s43588-024-00645-0

$B : m \in [-0.6, -0.7]$ $\quad$ $\{ \text{AND } h_B(x_i(t=T)) = 1$ $\quad$ $= 0$ otherwise

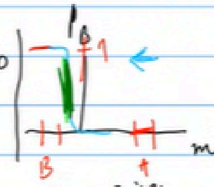
$\{ h_B(x) = 1$ if $x \in B$
$= 0$ otherwise

$A \cap B = \phi$



$\} \; p_B = 0$

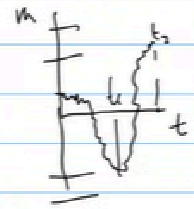
$\} \; p_B = 1$



Commitment prob. $p_B(x_0) \equiv$ prob. $\{ X_i(t=0) = X_0$ given, $h_B(x_i(t)) = 1 \rightarrow t_1$

$h_A(x_i(t)) = 1 \rightarrow t_2$

$t_1 < t_2 \}$



$\boxed{p_B(x) \rightarrow q(x)}$

$p(x) \propto e^{-\beta}$

ML: minimize for $\sum_{x \in \text{Boltzmann distribution}} |\nabla q|^2$

https://arxiv.org/pdf/2401.05279